Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 02:00 PM BST

PDB ID	:	4L3O
Title	:	Crystal Structure of SIRT2 in complex with the macrocyclic peptide S2iL5
Authors	:	Yamagata, K.; Nishimasu, H.; Ishitani, R.; Nureki, O.
Deposited on	:	2013-06-06
Resolution	:	2.52 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

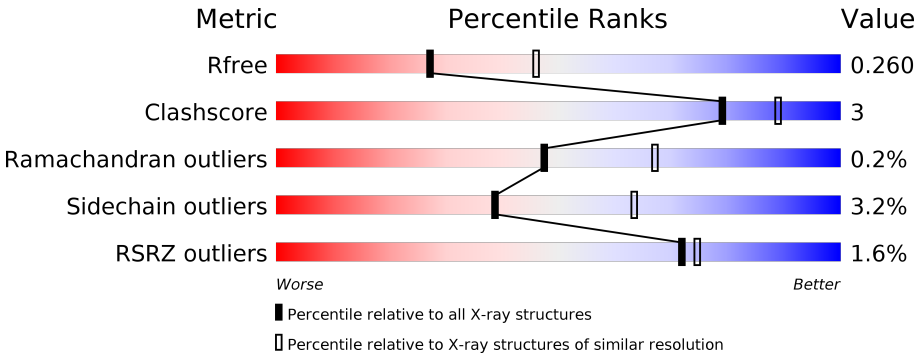
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	302	93% 5%
1	B	302	87% 11%
1	C	302	4% 87% 10%
1	D	302	85% 11%
2	E	16	88% 13%
2	F	16	81% 19%

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Mol	Chain	Length	Quality of chain
2	G	16	
2	H	16	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10482 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NAD-dependent protein deacetylase sirtuin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	1	0
			2368	1520	393	436	19			
1	B	295	Total	C	N	O	S	0	0	0
			2329	1497	388	425	19			
1	C	294	Total	C	N	O	S	0	0	0
			2320	1491	387	423	19			
1	D	293	Total	C	N	O	S	0	0	0
			2314	1485	383	427	19			

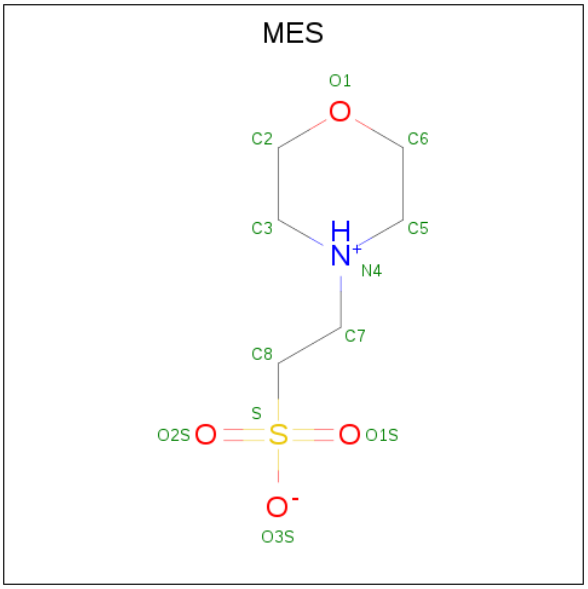
- Molecule 2 is a protein called cyclic peptide S2iL5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	16	Total	C	F	N	O	S	0	0	1
			144	90	3	27	23	1			
2	F	16	Total	C	F	N	O	S	0	0	1
			144	90	3	27	23	1			
2	G	16	Total	C	F	N	O	S	0	0	1
			144	90	3	27	23	1			
2	H	16	Total	C	F	N	O	S	0	0	1
			144	90	3	27	23	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

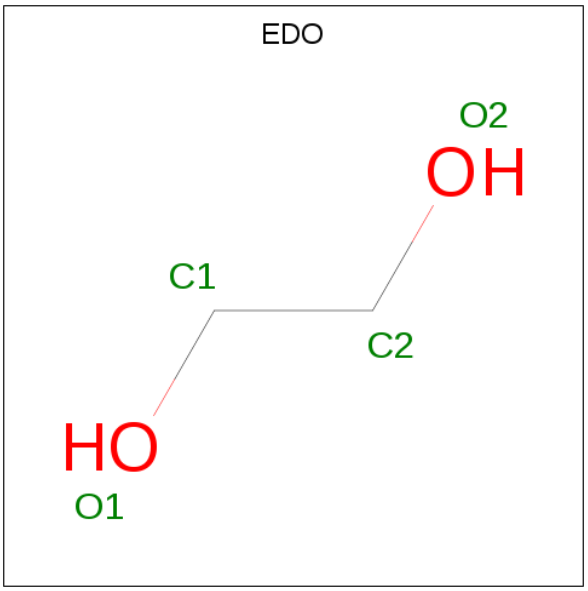
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

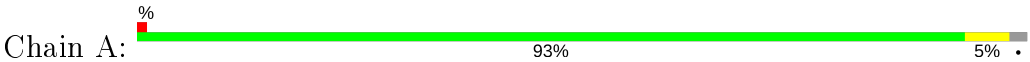
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	132	Total O 132 132	0	0
6	B	103	Total O 103 103	0	0
6	C	122	Total O 122 122	0	0
6	D	96	Total O 96 96	0	0
6	E	17	Total O 17 17	0	0
6	F	15	Total O 15 15	0	0
6	G	12	Total O 12 12	0	0
6	H	10	Total O 10 10	0	0

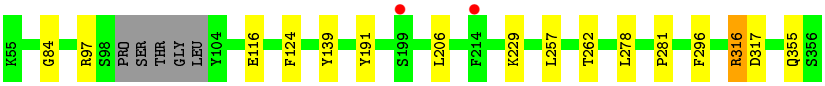
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NAD-dependent protein deacetylase sirtuin-2

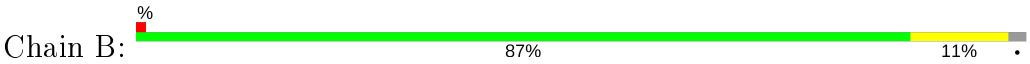
Chain A:

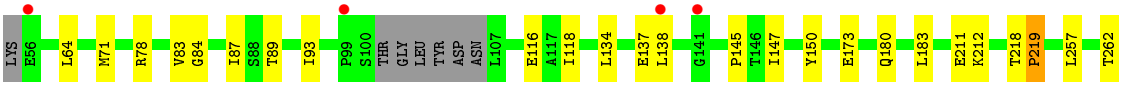


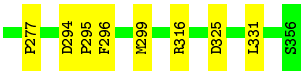


- Molecule 1: NAD-dependent protein deacetylase sirtuin-2

Chain B:

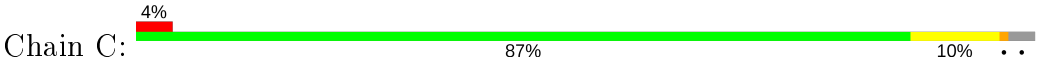


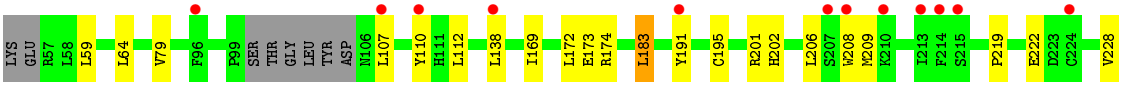




- Molecule 1: NAD-dependent protein deacetylase sirtuin-2

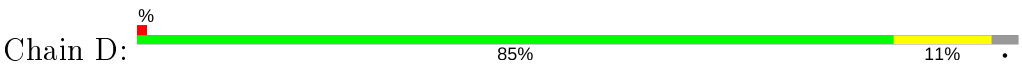
Chain C:

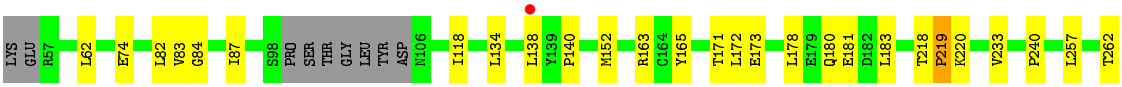


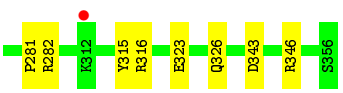


- Molecule 1: NAD-dependent protein deacetylase sirtuin-2

Chain D:

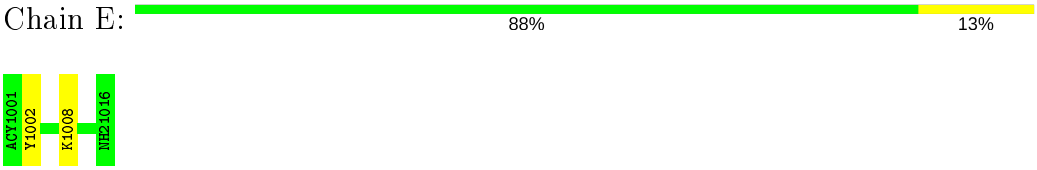






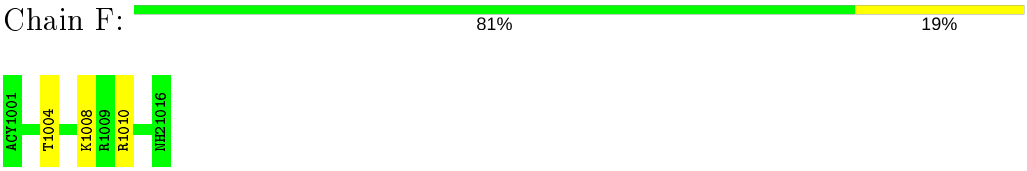
• Molecule 2: cyclic peptide S2iL5

Chain E:



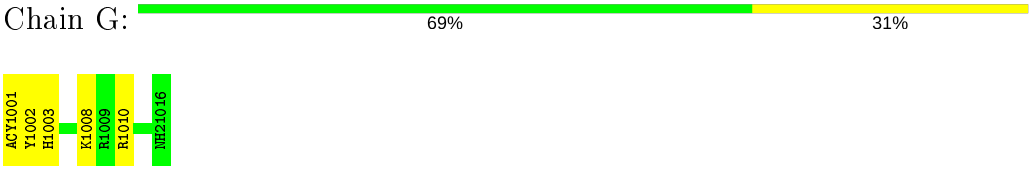
• Molecule 2: cyclic peptide S2iL5

Chain F:



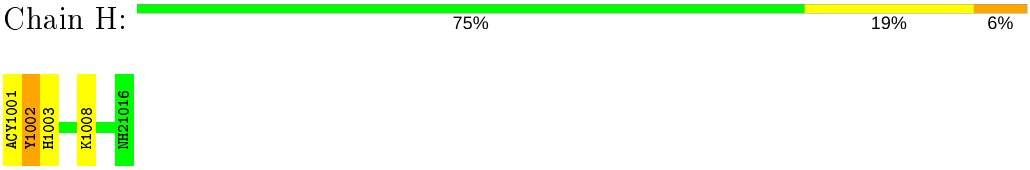
• Molecule 2: cyclic peptide S2iL5

Chain G:



• Molecule 2: cyclic peptide S2iL5

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.18Å 135.61Å 148.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.59 – 2.52 46.59 – 2.52	Depositor EDS
% Data completeness (in resolution range)	97.1 (46.59-2.52) 97.1 (46.59-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.211 , 0.263 0.207 , 0.260	Depositor DCC
R_{free} test set	6136 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 35.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10482	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EDO, FAK, MES, NH2, ACY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.22	0/2425	0.37	0/3269
1	B	0.22	0/2383	0.37	0/3215
1	C	0.22	0/2374	0.38	0/3204
1	D	0.22	0/2367	0.37	0/3195
2	E	0.22	0/129	0.42	0/173
2	F	0.22	0/129	0.38	0/173
2	G	0.23	0/129	0.42	0/173
2	H	0.25	0/129	0.42	0/173
All	All	0.22	0/10065	0.37	0/13575

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2368	0	2353	6	0
1	B	2329	0	2314	14	0
1	C	2320	0	2303	14	0
1	D	2314	0	2286	15	0
2	E	144	0	121	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	144	0	121	2	0
2	G	144	0	121	2	0
2	H	144	0	120	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	12	0	0
4	B	12	0	12	1	0
4	C	12	0	12	0	0
4	D	12	0	12	1	0
5	B	4	0	6	1	0
5	C	8	0	12	0	0
5	G	4	0	6	1	0
6	A	132	0	0	0	0
6	B	103	0	0	0	0
6	C	122	0	0	1	0
6	D	96	0	0	0	0
6	E	17	0	0	0	0
6	F	15	0	0	0	0
6	G	12	0	0	0	0
6	H	10	0	0	0	0
All	All	10482	0	9811	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:ASP:OD1	1:D:346:ARG:NH2	2.27	0.68
2:G:1010:ARG:H	5:G:1101:EDO:H22	1.59	0.67
1:C:138:LEU:HD21	1:C:169:ILE:HG13	1.81	0.62
1:D:257:LEU:HB2	1:D:282:ARG:HG2	1.83	0.60
1:B:71:MET:HE3	1:B:331:LEU:HD11	1.84	0.59
1:D:323:GLU:HB2	1:D:326:GLN:HG2	1.85	0.57
1:C:219:PRO:HB2	1:C:228:VAL:HB	1.88	0.56
1:C:308:ASP:OD1	1:C:311:SER:HB3	2.08	0.54
1:C:323:GLU:HB2	1:C:326:GLN:HG2	1.90	0.53
1:C:257:LEU:HB2	1:C:282:ARG:HG2	1.91	0.53
2:H:1001:ACY:C	2:H:1003:HIS:H	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:PRO:O	1:B:316:ARG:NH1	2.43	0.52
1:A:84:GLY:HA3	1:A:262:THR:HB	1.91	0.52
1:B:118:ILE:HD13	1:B:134:LEU:HD13	1.91	0.52
1:C:209:MET:HE1	1:C:219:PRO:HG3	1.91	0.51
1:D:233:VAL:HG21	1:D:240:PRO:HD3	1.93	0.51
1:C:79:VAL:HG22	1:C:256:LEU:HB3	1.93	0.51
1:A:191:TYR:HA	1:A:206:LEU:HD13	1.93	0.50
2:H:1001:ACY:O	2:H:1003:HIS:N	2.35	0.50
1:C:338:LYS:HB3	1:C:339:LYS:HE3	1.92	0.50
1:B:116:GLU:HG3	2:F:1010:ARG:HH21	1.76	0.49
1:C:174:ARG:NH2	6:C:683:HOH:O	2.46	0.48
1:B:147:ILE:HD12	1:B:325:ASP:HB3	1.96	0.48
1:D:62:LEU:HD21	1:D:315:TYR:O	2.14	0.47
2:H:1001:ACY:O	2:H:1003:HIS:ND1	2.47	0.47
1:C:195:CYS:HB3	1:C:201:ARG:HA	1.96	0.47
1:D:83:VAL:HB	1:D:87:ILE:HD13	1.97	0.47
1:D:281:PRO:HA	1:D:316:ARG:HB2	1.98	0.46
1:B:83:VAL:HB	1:B:87:ILE:HD13	1.96	0.46
1:C:191:TYR:HA	1:C:206:LEU:HD12	1.98	0.46
1:D:82:LEU:HD23	1:D:165:TYR:HB2	1.99	0.45
1:D:163:ARG:NH1	1:D:181:GLU:O	2.49	0.44
1:C:110:TYR:HB2	1:C:112:LEU:HG	1.99	0.44
1:B:299:MET:HE1	2:F:1004:THR:H	1.82	0.44
1:B:294:ASP:HA	1:B:295:PRO:HD3	1.89	0.43
1:D:118:ILE:HD13	1:D:134:LEU:HD13	2.00	0.43
2:G:1001:ACY:C	2:G:1003:HIS:H	2.29	0.43
1:B:212:LYS:HD3	1:B:219:PRO:HA	2.01	0.42
1:B:78:ARG:HG2	5:B:503:EDO:H21	2.00	0.42
1:A:97:ARG:NH2	1:A:116:GLU:OE1	2.53	0.42
1:A:281:PRO:HA	1:A:316:ARG:HB2	2.01	0.42
1:B:84:GLY:HA3	1:B:262:THR:HB	2.02	0.42
1:C:173:GLU:HB2	1:C:183:LEU:HD21	2.02	0.42
1:D:173:GLU:O	1:D:178:LEU:HB2	2.20	0.42
1:D:218:THR:HA	1:D:219:PRO:HD3	1.87	0.41
1:B:218:THR:HA	1:B:219:PRO:HD3	1.94	0.41
4:D:502:MES:H51	4:D:502:MES:H81	1.87	0.41
1:A:316:ARG:HD2	1:A:317:ASP:OD1	2.20	0.41
4:B:502:MES:H51	4:B:502:MES:H81	1.74	0.41
1:C:208:TRP:HH2	1:C:222:GLU:HG2	1.86	0.40
1:D:84:GLY:HA3	1:D:262:THR:HB	2.02	0.40
1:A:124:PHE:CE2	1:A:229:LYS:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:PRO:HB2	1:B:150:TYR:CE2	2.56	0.40
1:B:89:THR:HA	1:B:93:ILE:O	2.21	0.40
1:D:62:LEU:HD21	1:D:315:TYR:C	2.42	0.40
1:D:140:PRO:HB3	1:D:171:THR:OG1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	294/302 (97%)	288 (98%)	6 (2%)	0	100 100
1	B	291/302 (96%)	286 (98%)	4 (1%)	1 (0%)	41 59
1	C	290/302 (96%)	280 (97%)	10 (3%)	0	100 100
1	D	289/302 (96%)	279 (96%)	9 (3%)	1 (0%)	41 59
2	E	13/16 (81%)	10 (77%)	3 (23%)	0	100 100
2	F	13/16 (81%)	11 (85%)	2 (15%)	0	100 100
2	G	13/16 (81%)	11 (85%)	2 (15%)	0	100 100
2	H	13/16 (81%)	11 (85%)	1 (8%)	1 (8%)	1 1
All	All	1216/1272 (96%)	1176 (97%)	37 (3%)	3 (0%)	47 67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	1002	TYR
1	D	219	PRO
1	B	219	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	259/263 (98%)	253 (98%)	6 (2%)	50	74
1	B	253/263 (96%)	244 (96%)	9 (4%)	35	59
1	C	252/263 (96%)	243 (96%)	9 (4%)	35	59
1	D	252/263 (96%)	245 (97%)	7 (3%)	43	68
2	E	13/13 (100%)	12 (92%)	1 (8%)	13	23
2	F	13/13 (100%)	13 (100%)	0	100	100
2	G	13/13 (100%)	12 (92%)	1 (8%)	13	23
2	H	13/13 (100%)	12 (92%)	1 (8%)	13	23
All	All	1068/1104 (97%)	1034 (97%)	34 (3%)	39	63

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	TYR
1	A	257	LEU
1	A	278	LEU
1	A	296	PHE
1	A	316	ARG
1	A	355	GLN
1	B	64	LEU
1	B	137	GLU
1	B	138	LEU
1	B	173	GLU
1	B	180	GLN
1	B	183	LEU
1	B	211	GLU
1	B	257	LEU
1	B	296	PHE
1	C	59	LEU
1	C	64	LEU
1	C	107	LEU
1	C	172	LEU

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Mol	Chain	Res	Type
1	C	183	LEU
1	C	202	HIS
1	C	296	PHE
1	C	311	SER
1	C	339	LYS
1	D	74	GLU
1	D	138	LEU
1	D	152	MET
1	D	172	LEU
1	D	180	GLN
1	D	183	LEU
1	D	220	LYS
2	E	1002	TYR
2	G	1002	TYR
2	H	1002	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	GLN
1	A	225	GLN
1	A	326	GLN
1	B	194	HIS
1	B	202	HIS
1	C	142	GLN
1	C	355	GLN
1	D	167	GLN
1	D	180	GLN
1	D	202	HIS
1	D	326	GLN
2	F	1006	HIS
2	G	1006	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAK	G	1008	2	13,14,15	1.73	2 (15%)	13,18,20	1.84	1 (7%)
2	FAK	F	1008	2	13,14,15	1.70	2 (15%)	13,18,20	1.56	1 (7%)
2	FAK	H	1008	2	13,14,15	1.73	2 (15%)	13,18,20	1.56	1 (7%)
2	FAK	E	1008	2	13,14,15	1.70	2 (15%)	13,18,20	1.97	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAK	G	1008	2	-	1/15/16/18	-
2	FAK	F	1008	2	-	4/15/16/18	-
2	FAK	H	1008	2	-	5/15/16/18	-
2	FAK	E	1008	2	-	0/15/16/18	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1008	FAK	CH-NZ	4.76	1.43	1.34
2	F	1008	FAK	CH-NZ	4.67	1.43	1.34
2	G	1008	FAK	CH-NZ	4.65	1.43	1.34
2	H	1008	FAK	CH-NZ	4.62	1.43	1.34
2	H	1008	FAK	CB-CA	-3.23	1.49	1.53
2	G	1008	FAK	CB-CA	-3.18	1.49	1.53
2	F	1008	FAK	CB-CA	-3.07	1.49	1.53
2	E	1008	FAK	CB-CA	-2.93	1.49	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1008	FAK	CT-CH-NZ	6.15	120.63	115.25
2	G	1008	FAK	CT-CH-NZ	5.60	120.15	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1008	FAK	CT-CH-NZ	4.70	119.36	115.25
2	H	1008	FAK	CT-CH-NZ	4.63	119.30	115.25

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1008	FAK	NZ-CH-CT-FI2
2	H	1008	FAK	NZ-CH-CT-FI1
2	H	1008	FAK	NZ-CH-CT-FI3
2	F	1008	FAK	NZ-CH-CT-FI1
2	F	1008	FAK	NZ-CH-CT-FI3
2	H	1008	FAK	OH-CH-CT-FI1
2	H	1008	FAK	OH-CH-CT-FI3
2	G	1008	FAK	NZ-CH-CT-FI2
2	H	1008	FAK	NZ-CH-CT-FI2
2	F	1008	FAK	OH-CH-CT-FI2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EDO	B	503	-	3,3,3	0.46	0	2,2,2	0.28	0
4	MES	A	502	-	12,12,12	2.30	1 (8%)	14,16,16	2.06	6 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	C	504	-	3,3,3	0.48	0	2,2,2	0.29	0
5	EDO	G	1101	-	3,3,3	0.45	0	2,2,2	0.35	0
5	EDO	C	503	-	3,3,3	0.47	0	2,2,2	0.27	0
4	MES	C	502	-	12,12,12	2.29	1 (8%)	14,16,16	2.20	7 (50%)
4	MES	B	502	-	12,12,12	2.24	1 (8%)	14,16,16	1.95	6 (42%)
4	MES	D	502	-	12,12,12	2.27	1 (8%)	14,16,16	2.02	7 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	503	-	-	0/1/1/1	-
4	MES	A	502	-	-	1/6/14/14	0/1/1/1
5	EDO	C	504	-	-	0/1/1/1	-
5	EDO	G	1101	-	-	0/1/1/1	-
5	EDO	C	503	-	-	0/1/1/1	-
4	MES	C	502	-	-	1/6/14/14	0/1/1/1
4	MES	B	502	-	-	0/6/14/14	0/1/1/1
4	MES	D	502	-	-	1/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	MES	C8-S	-7.70	1.66	1.77
4	C	502	MES	C8-S	-7.65	1.66	1.77
4	D	502	MES	C8-S	-7.57	1.66	1.77
4	B	502	MES	C8-S	-7.48	1.66	1.77

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	502	MES	C5-N4-C3	4.54	119.05	108.83
4	C	502	MES	C5-N4-C3	4.22	118.34	108.83
4	D	502	MES	C5-N4-C3	4.19	118.26	108.83
4	B	502	MES	C5-N4-C3	4.00	117.84	108.83
4	C	502	MES	C6-C5-N4	-3.70	104.49	110.10
4	D	502	MES	C6-C5-N4	-3.00	105.56	110.10
4	A	502	MES	C6-C5-N4	-2.87	105.75	110.10
4	B	502	MES	C6-C5-N4	-2.85	105.79	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	502	MES	C7-N4-C3	2.71	118.17	111.23
4	C	502	MES	C7-N4-C5	2.60	117.89	111.23
4	A	502	MES	O1S-S-C8	2.49	109.91	106.92
4	C	502	MES	O3S-S-C8	2.47	109.77	105.77
4	A	502	MES	O3S-S-C8	2.40	109.64	105.77
4	B	502	MES	O2S-S-C8	2.36	109.75	106.92
4	C	502	MES	O1S-S-C8	2.36	109.75	106.92
4	A	502	MES	C7-N4-C3	2.33	117.19	111.23
4	D	502	MES	O3S-S-C8	2.32	109.52	105.77
4	A	502	MES	C7-N4-C5	2.31	117.14	111.23
4	D	502	MES	O1S-S-C8	2.28	109.66	106.92
4	C	502	MES	C2-C3-N4	-2.26	106.67	110.10
4	D	502	MES	C7-N4-C5	2.25	116.99	111.23
4	B	502	MES	O1S-S-C8	2.21	109.58	106.92
4	B	502	MES	O3S-S-C8	2.20	109.32	105.77
4	B	502	MES	C7-N4-C5	2.14	116.70	111.23
4	D	502	MES	C7-N4-C3	2.10	116.61	111.23
4	D	502	MES	O2S-S-C8	2.05	109.38	106.92

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	MES	C8-C7-N4-C3
4	C	502	MES	C8-C7-N4-C3
4	D	502	MES	C8-C7-N4-C3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	503	EDO	1	0
5	G	1101	EDO	1	0
4	B	502	MES	1	0
4	D	502	MES	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	297/302 (98%)	-0.38	2 (0%) 87 89	13, 25, 58, 71	0
1	B	295/302 (97%)	-0.11	4 (1%) 75 78	15, 38, 70, 101	0
1	C	294/302 (97%)	-0.11	12 (4%) 37 41	12, 29, 73, 91	0
1	D	293/302 (97%)	-0.14	2 (0%) 87 89	17, 42, 65, 82	0
2	E	13/16 (81%)	-0.40	0 100 100	15, 20, 26, 27	0
2	F	13/16 (81%)	-0.11	0 100 100	16, 19, 26, 26	0
2	G	13/16 (81%)	-0.24	0 100 100	15, 23, 29, 29	0
2	H	13/16 (81%)	-0.10	0 100 100	17, 24, 32, 37	0
All	All	1231/1272 (96%)	-0.19	20 (1%) 72 74	12, 32, 67, 101	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	110	TYR	4.2
1	C	214	PHE	3.7
1	B	99	PRO	3.6
1	C	210	LYS	3.2
1	C	107	LEU	3.0
1	C	215	SER	3.0
1	C	208	TRP	2.9
1	C	138	LEU	2.8
1	C	213	ILE	2.7
1	C	191	TYR	2.5
1	B	141	GLY	2.5
1	B	56	GLU	2.5
1	C	207	SER	2.3
1	D	138	LEU	2.3
1	D	312	LYS	2.3
1	C	224	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	96	PHE	2.2
1	A	214	PHE	2.1
1	B	138	LEU	2.1
1	A	199	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAK	G	1008	15/16	0.95	0.15	11,20,27,29	0
2	FAK	F	1008	15/16	0.96	0.14	15,18,32,39	0
2	FAK	H	1008	15/16	0.97	0.11	16,23,36,37	0
2	FAK	E	1008	15/16	0.97	0.12	10,15,23,30	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	C	501	1/1	0.89	0.07	70,70,70,70	0
5	EDO	B	503	4/4	0.93	0.14	35,36,42,42	0
4	MES	A	502	12/12	0.93	0.21	35,59,64,67	0
5	EDO	C	503	4/4	0.93	0.17	24,28,29,38	0
4	MES	D	502	12/12	0.94	0.22	47,55,67,74	0
4	MES	C	502	12/12	0.95	0.14	40,52,63,68	0
4	MES	B	502	12/12	0.95	0.19	38,58,68,72	0
3	ZN	D	501	1/1	0.95	0.04	58,58,58,58	0
5	EDO	G	1101	4/4	0.96	0.14	27,33,34,37	0
5	EDO	C	504	4/4	0.96	0.39	30,31,40,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	A	501	1/1	0.98	0.04	66,66,66,66	0
3	ZN	B	501	1/1	0.99	0.07	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.